

and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 10:10:21 ON 24 JUN 2009

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.22

0.22

FILE 'REGISTRY' ENTERED AT 10:10:40 ON 24 JUN 2009

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 22 JUN 2009 HIGHEST RN 1159446-15-7

DICTIONARY FILE UPDATES: 22 JUN 2009 HIGHEST RN 1159446-15-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

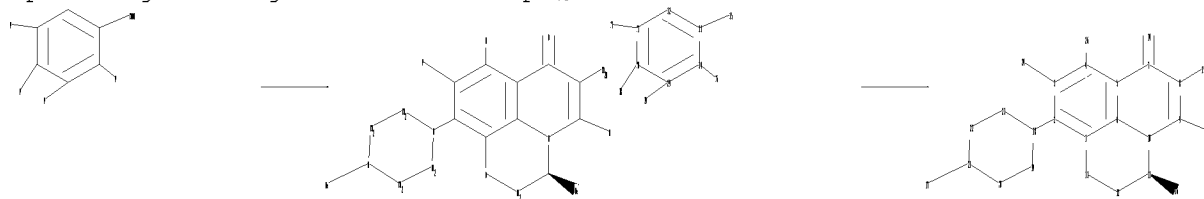
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10578078cc.str



chain nodes :  
14 15 16 17 24 25 26 35 36 37 38 39  
ring nodes :

```

1  2  3  4  5  6  7  8  9 10 11 12 13 18 19 20 21 22 23 29 30 31 32
33 34
chain bonds :
2-18  3-24  4-26  7-14  8-15  9-25 11-16 17-21 29-39 30-38 31-37 33-35 34-36

ring bonds :
1-2  1-6  1-13  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10 10-11 11-12 12-13
18-19 18-23 19-20 20-21 21-22 22-23 29-30 29-34 30-31 31-32 32-33 33-34
exact/norm bonds :
1-13  2-18  5-7  6-10  7-8  7-14  8-9  9-10 10-11 11-12 12-13 18-19 18-23
19-20 20-21 21-22 22-23
exact bonds :
3-24  4-26  8-15  9-25 11-16 17-21 29-39 30-38 31-37 33-35 34-36
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  29-30 29-34 30-31 31-32 32-33 33-34

```

## Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 29:CLASS
30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:CLASS 36:CLASS 37:CLASS 38:CLASS
39:CLASS

```

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

containing 29

## Stereo Bonds:

16-11 (Single Wedge).

## Stereo Chiral Centers:

11 (Parity=Don't Care)

## Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 11

L1 STRUCTURE UPLOADED

=&gt; d 11

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=&gt; file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.48

0.70

FILE 'CASREACT' ENTERED AT 10:11:11 ON 24 JUN 2009  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 21 Jun 2009 VOL 150 ISS 26

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*      CASREACT now has more than 16.5 million reactions
*
*****
```

CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l1

SAMPLE SEARCH INITIATED 10:11:16 FILE 'CASREACT'  
SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS  
  
100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 0 TO 0  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s l1 sss full

FULL SEARCH INITIATED 10:11:23 FILE 'CASREACT'  
SCREENING COMPLETE - 115 REACTIONS TO VERIFY FROM 10 DOCUMENTS  
  
100.0% DONE 115 VERIFIED 8 HIT RXNS 3 DOCS  
SEARCH TIME: 00.00.02

L3 3 SEA SSS FUL L1 ( 8 REACTIONS)

=> d ibib abs fhit tot

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 144:468205 CASREACT  
 TITLE: Synthetic process for the preparation of levofloxacin hemihydrate from levofloxacin  
 INVENTOR(S): Rao, Davuluri Rammohan; Dwivedi, Shripakash Dhar; Sreenivasulu, Pamujula; Sahu, Arabinda; Trinadhachari, Ganala Naga; Kiran, Surapaneni Sasi  
 PATENT ASSIGNEE(S): Neuland Laboratories Ltd., India  
 SOURCE: PCT Int. Appl., 31 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006048889	A1	20060511	WO 2004-IN343	20041108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM US 20070244318 A1 20071018 US 2004-578078 20040811 EP 1809637 A1 20070725 EP 2004-806742 20041108 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR PRIORITY APPLN. INFO.: WO 2004-IN343 20041108 AB A process for preparation of Levofloxacin hemihydrate, having single individual impurity not more than 0.1% and free from particulate matter and from the other enantiomer (R-form), is described which comprises: dissolving levofloxacin tech. grade in an aqueous alkaline solution; treating the solution with activated carbon at room temperature; removing the undissolved particulate matter by filtration; bringing the pH of the aqueous alkaline levofloxacin solution to neutral using dilute mineral acid; removing the precipitated particulate matter by filtration; acidifying the resulting solution; treating the acidified solution with activated carbon at room temperature; filtering the undissolved particulate matter by filtration; neutralizing the acidic solution; filtering again to remove any particulate matter present; and extracting the resulting product with a chlorinated solvent (e.g., Cl <sub>2</sub> CH <sub>2</sub> ) and concentrating under vacuum				

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
 PRO B 94695-48-4  
 SOL 68-12-2 DMF  
 CON SUBSTAGE(1) room temperature -> 90 deg C  
 SUBSTAGE(2) 6 - 8 hours

RX(2) RCT E 105-53-3  
 STAGE(1)  
 SOL 64-17-5 EtOH, 108-88-3 PhMe  
 CON 20 minutes, room temperature  
 STAGE(2)  
 RGT G 7439-95-4 Mg  
 CAT 67-66-3 CHCl<sub>3</sub>  
 SOL 64-17-5 EtOH  
 CON SUBSTAGE(1) room temperature  
 SUBSTAGE(2) 30 minutes, room temperature  
 SUBSTAGE(3) 3 - 4 hours, 70 - 90 deg C  
 SUBSTAGE(4) 2 hours, 70 - 90 deg C  
 SUBSTAGE(5) 90 deg C -> 55 deg C  
 STAGE(3)  
 RCT B 94695-48-4  
 SOL 109-99-9 THF, 108-88-3 PhMe  
 CON SUBSTAGE(2) 30 - 35 deg C  
 SUBSTAGE(3) 35 deg C -> 5 deg C  
 SUBSTAGE(4) - 2 hour, 0 - 5 deg C  
 SUBSTAGE(5) 30 minutes, 0 - 5 deg C  
 SUBSTAGE(6) 5 deg C -> 25 deg C  
 SUBSTAGE(7) 30 minutes, 20 - 25 deg C

PRO F 94695-49-5  
 RX(3) RCT F 94695-49-5  
 RGT M 104-15-4 TsOH  
 PRO L 94695-50-8  
 SOL 7732-18-5 Water  
 CON 3 hours, 80 - 90 deg C

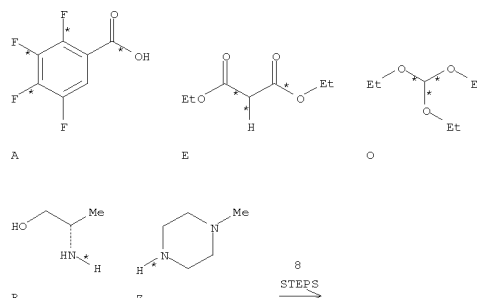
RX(4) RCT L 94695-50-8, O 122-51-0  
 PRO F 94714-58-6  
 SOL 108-24-7 Ac<sub>2</sub>O  
 CON SUBSTAGE(1) room temperature -> 125 deg C  
 SUBSTAGE(2) 4 hours, 120 - 125 deg C

RX(5) RCT P 94714-58-6, R 2749-11-3  
 PRO S 110548-02-2  
 SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>  
 CON SUBSTAGE(1) 30 - 35 deg C  
 SUBSTAGE(2) 35 deg C -> 5 deg C  
 SUBSTAGE(3) - 2 hour, 0 - 5 deg C  
 SUBSTAGE(4) 5 deg C -> 35 deg C  
 SUBSTAGE(5) 2 hours, 30 - 35 deg C

RX(6) RCT S 110548-02-2  
 RGT V 584-08-7 K<sub>2</sub>CO<sub>3</sub>  
 PRO U 106939-34-8  
 SOL 68-12-2 DMF

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
 using aq. THF or an admixt. with other org. solvents to get highly pure levofloxacin hemihydrate having a single individual impurity which is <0.1% and is free from particulate matter and from the other enantiomer (R-form).

RX(36) OF 36 COMPOSED OF RX(1), RX(2), RX(3), RX(4), RX(5), RX(6), RX(7), RX(8)  
 RX(36) A + E + O + R + Z ==> AA



AA  
 RX(1) RCT A 1201-31-6  
 RGT C 7719-09-7 SOCl<sub>2</sub>

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
 CON SUBSTAGE(1) 120 deg C  
 SUBSTAGE(2) 2 hours, 120 deg C  
 SUBSTAGE(3) 30 minutes

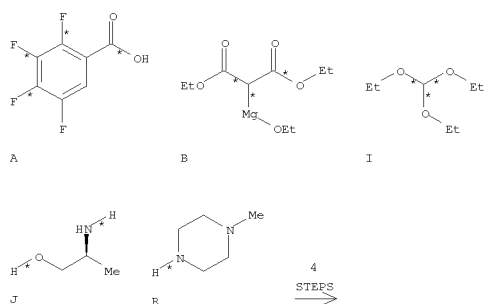
RX(7) RCT U 106939-34-8  
 RGT X 7647-01-0 HCl  
 PRO W 100986-89-8  
 SOL 7732-18-5 Water, 64-19-7 AcOH  
 CON SUBSTAGE(1) room temperature -> 80 deg C  
 SUBSTAGE(2) 6 hours, 75 - 80 deg C  
 SUBSTAGE(3) 80 deg C -> 20 deg C  
 SUBSTAGE(4) 1 hour, 15 - 20 deg C

RX(8) RCT W 100986-89-8, Z 109-01-3  
 RGT AB 110-86-1 Pyridine  
 PRO AA 100986-85-4  
 SOL 110-86-1 Pyridine  
 CON 10 hours, room temperature -> 120 deg C

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE  
 FORMAT

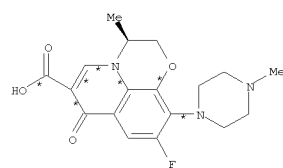
L3 ANSWER 2 OF 3 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 135:107303 CASREACT  
 TITLE: Studies on stereospecific synthesis of  
 (S)-(-)-ofloxacin  
 AUTHOR(S): Li, Jiaming; Wang, Gang; Zhang, Xing; Zhou, Sixiang  
 CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Anhui College  
 of Traditional Chinese Medicines, Hefei, 230038,  
 Peop.  
 SOURCE: Rep. China  
 Zhongguo Yaowu Huaxue Zazhi (2000), 10(4), 276-278  
 CODEN: ZYHZEJ; ISSN: 1005-0108  
 PUBLISHER: Zhongguo Yaowu Huaxue Zazhi Bianjibu  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Chinese  
 AB (S)-(-)-Ofloxacin was synthesized from 2,3,4,5- tetrafluorobenzoic acid  
 by  
 chlorination, condensation with di-Et malonate, partial hydrolysis,  
 decarboxylation, condensation with tri-Et orthoformate, substitution with  
 (S)-(+)-2-aminopropanol, cyclization, hydrolysis, and substitution with  
 N-methylpiperazine. The overall yield from 2,3,4,5-tetrafluorobenzoic  
 acid was 39.2%.

RX(10) OF 10 COMPOSED OF RX(1), RX(2), RX(3), RX(4)  
 RX(10) A + B + I + J + R ==> S



L3 ANSWER 2 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
 RX(4) RCT R 109-01-3, O 100986-89-8  
 PRO S 100986-85-4  
 SOL 67-68-5 DMSO

L3 ANSWER 2 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

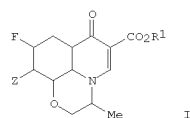


S  
 YIELD 82%

RX(1) RCT A 1201-31-6  
 STAGE(1)  
 RGT D 7719-09-7 SOC12  
 SOL 68-12-2 DMF  
 STAGE(2)  
 RCT B 207746-86-9  
 SOL 108-88-3 PhMe  
 STAGE(3)  
 RGT E 104-15-4 TsOH  
 SOL 7732-18-5 Water  
 PRO C 94695-50-8  
 RX(2) RCT I 122-51-0, C 94695-50-8  
 STAGE(1)  
 SOL 108-24-7 Ac2O  
 STAGE(2)  
 RCT J 2749-11-3  
 SOL 75-09-2 CH2Cl2  
 STAGE(3)  
 RGT L 584-08-7 K2CO3  
 SOL 68-12-2 DMF  
 PRO K 106939-34-8  
 RX(3) RCT K 106939-34-8  
 RGT P 7647-01-0 HCl  
 PRO O 100986-89-8  
 SOL 64-19-7 AcOH

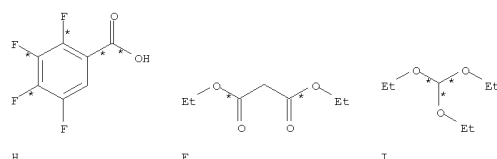
L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2009 ACS on STN  
 ACCESSION NUMBER: 110:75530 CASREACT  
 TITLE: Process for preparation of racemic and optically  
 active ofloxacin and related derivatives  
 INVENTOR(S): Mitscher, Lester A.; Chu, Daniel T.  
 PATENT ASSIGNEE(S): Abbott Laboratories, USA  
 SOURCE: U.S., 7 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4777253	A	19881011	US 1986-858532	19860425
US 4826985	A	19890502	US 1988-216063	19880707
PRIORITY APPLN. INFO.:			US 1986-858532	19860425
OTHER SOURCE(S):			MARPAT 110:75530	
GI				



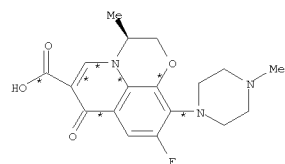
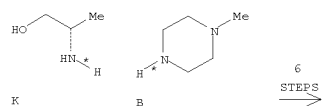
AB The title compds. I (R1 = H, C1-4 alkyl, PhCH2; Z = R4R5N; R4, R5 = H,  
 alkanoyl, alkanoylamido, substituted amino; R4R5N = (un)substituted  
 aliphatic  
 heterocyclyl) (wherein the the racemate of ofloxacin exhibits  
 antibacterial properties) were prepared (-)-I (R1 = Et; Z = F)  
 (preparation  
 given) in pyridine was added to 1-methylpiperazine, the mixture heated to  
 55°, and after workup, the solid obtained was dissolved in THF and  
 NaOH solution to give (-)-I (R1 = H; Z = 4-methylpiperazinyl).

RX(86) OF 102 COMPOSED OF RX(4), RX(3), RX(5), RX(6), RX(13), RX(9)  
 RX(86) H + F + I + K + B ==> N



L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



N

RX(4) RCT H 1201-31-6  
PRO E 94695-48-4

RX(3) RCT E 94695-48-4, F 105-53-3  
PRO G 94695-50-8

RX(5) RCT G 94695-50-8, I 122-51-0  
PRO J 94714-58-6

RX(6) RCT J 94714-58-6, K 2749-11-3  
PRO L 110548-02-2

RX(13) RCT L 110548-02-2  
PRO P 106939-34-8  
SOL 109-99-9 THF

RX(9) RCT P 106939-34-8, B 109-01-3  
RGT Q 7732-18-5 Water  
PRO N 100986-85-4  
SOL 7732-18-5 Water

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT